

Abstract Submitted
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Transport Properties in Carbon Nanotubes films for Hydrogen Sensor Applications¹ JIANWEI ZHANG, YAO HE, CHAO CAO, LEX KEMPER, HAI-PING CHENG, Department of Physics and Quantum Theory Project, University of Florida — Thin single-walled carbon nanotube (CNT) films doped with palladium (Pd) on surface are shown to be promising in hydrogen(H₂) sensor applications. We study electronic transport properties of CNT/Pd/H₂ system by combining first-principles band structure calculations with Boltzmann transport theory. The coupling between Pd atoms and carbon nanotubes is described by the Kondo model. An effective scattering potential, which creates the major resistance in nanotubes, is calculated by fitting potential parameters to the calculated band structures. In addition, intersection resistance between the nanotubes is also included in our simulations. We will present the band structure of the CNT/Pd system with and without the hydrogen atoms or hydrogen molecules. The conductance change of the whole nanotube films in the presence of hydrogen gas will be shown.

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